checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pmn21

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: pmn21

```
Bond precision:   O- B = 0.0027 A          Wavelength=0.71073

Cell:               a=16.2527(4)       b=4.4373(1)      c=8.8174(2)
                    alpha=90           beta=90          gamma=90
Temperature:        298 K

                 Calculated                  Reported
Volume           635.89(3)                   635.89(3)
Space group      P m n 21                    P m n 21
Hall group       P 2ac -2                    P 2ac -2
Moiety formula   B10 H5 O22 Tb3              B10 H5 O22 Tb3
Sum formula      B10 H5 O22 Tb3              B10 H5 O22 Tb3
Mr               941.93                      941.90
Dx,g cm-3        4.919                       4.919
Z                2                           2
Mu (mm-1)        16.665                      16.664
F000             852.0                       852.0
F000'            851.59
h,k,lmax         29,7,15                     29,7,15
Nref             3894[ 2038]                 3859
Tmin,Tmax        0.454,0.607                 0.385,0.609
Tmin'            0.113

Correction method= # Reported T Limits: Tmin=0.385 Tmax=0.609
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.99        Theta(max)= 39.440

R(reflections)= 0.0110( 3850)                wR2(reflections)=
                                             0.0254( 3859)
S = 1.135                  Npar= 181
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ..... O13 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.63Ang From Tb1 -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.60Ang From Tb1 -1.66 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.995 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact B1 ..B4 . 2.64 Ang.
1/2-x,2-y,1/2+z = 2_575 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Tb1 (III) . 2.96 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Tb2 (III) . 2.66 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 4 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT953_ALERT_1_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock pmn21 - ellipsoid plot